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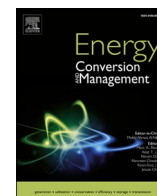
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The performance and efficiency of novel oxy-hydrogen-argon gas power cycles for zero emission power generation

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ABSTRACT

This study investigates the performance and efficiency of closed-loop oxy-hydrogen Brayton power cycles through numerical modelling and simulation. Coupled with storage hydrogen and oxygen produced by a water-electrolysis system, these cycles have the potential to produce flexible electrical power at high thermal efficiency whilst producing zero exhaust gas emissions. The efficiency and power output of the cycles are investigated using a thermodynamic model. A standard Argon Power Cycle (APC) fuelled by hydrogen is explored which yields an efficiency of 19% under typical operating conditions. To improve the performance, the cycle is modified by including an intercooler, reheater and regenerator, which has the potential to increase the efficiency to 64% when operating under the same conditions. In addition, the potential use of helium and air as the working fluid is explored, as well as a methane fuelled cycle. It is found that the hydrogen-helium cycle is more efficient over all pressure ratios but the most expensive to operate.

1. Introduction

In 2019, electricity generation contributed to 26% of the greenhouse gas (GHG) emissions in the United Kingdom (UK), making it the second largest emitting sector after transport [1]. To combat climate change, the UK has pledged net zero GHG emissions by 2050 [2]. With the expected increase in demand from transport and heating, the Committee on Climate Change predict low carbon electricity generation will need to quadruple to 645 TWh annually to meet this target [3].

A potential gateway to electrification is to use hydrogen gas storage to smooth the intermittency of renewable energy generation. During periods when the production of energy exceeds demand, excess energy is diverted to a water electrolyser which produces hydrogen and oxygen for compression and storage. By storing energy in hydrogen, it can be easily transported and remain stored indefinitely. As independent organisations such as the International Energy Agency [4] are suggesting there will be huge price reductions (30% by 2030 and > 50% by 2050) for water electrolysis installation costs as a result around a 80 times [5] scale up in installed capacity is expected by 2050. This means there will be an abundance of renewable hydrogen but also a proportional amount of co-produced oxygen.

When needed, the hydrogen can be recombined with oxygen and electricity or heat generated. This process is shown in Fig. 1 and has the

potential to have high round trip efficiencies whilst producing zero emissions.

1.1. Scope and potential opportunities for hydrogen

Compressed hydrogen has advantages over existing energy storage methods including high capacity, reliability, high energy density and rapid discharge rates. Fig. 2 shows hydrogen has the greatest potential for long term, large scale energy storage [6].

Whilst there is a focus on using hydrogen in fuel cells due to a high efficiency, similar levels of efficiencies can also be achieved in novel closed loop Argon Power Cycles (APC). One such cycle with potential is based on a linear Joule cycle which has been proposed by Durham University [7], a solution which aims to generate heat and electricity from stored hydrogen and oxygen. The use of argon as the working fluid rather than air raises the specific heat ratio (γ) from 1.4 to 1.613. Argon is a suitable choice because it is unreactive, abundant, easier to obtain than other noble gases and facilitates the creation of tight gas seals [8]. Using the ideal Brayton cycle efficiency equation, it can be expected that increasing γ will increase the theoretical efficiency (η) by around 11%. The ideal efficiency is also dependent on the temperature ratio (TR), which can be substituted for the pressure ratio (PR), as shown in Eq. (1).

$$\eta = 1 - \frac{1}{TR} = 1 - \frac{1}{PR^{(\gamma-1)/\gamma}} \quad (1)$$

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Nomenclature

Parameter Symbol

Argon Power Cycle	APC
Compressed Air Energy Storage	CAES
Higher Heating Value	HHV
Molar Flow Rate	MFR
Room Temperature and Pressure	RTP
Degrees of Freedom	DoF
Heat added from combustion (Watts)	Q_{in}
Fuel molar flow rate (kMol/s)	\dot{n}
Useful heat in coolant streams (Watts)	Q_c
Net power output (Watts)	W_{net}
Specific heat ratio (-)	γ
Specific heat at constant pressure (J/gK)	c_p
Ideal gas constant (J/kgK)	R

Work has been carried out to determine what effects the efficiency of APCs. Early research in this area was carried out by Kuroki et al. [8] in 2010. They investigated a number of scenarios that quantified the efficiency of an argon circulated, hydrogen fuelled, internal combustion engine. Steam is the only product of combustion and is extracted from the cycle in a condenser. However, residual steam that is not removed recirculates and can build up over time. As steam has a lower specific heat ratio than argon, its presence reduces the theoretical efficiency. Kuroki et al. found that the maximum efficiency reduction caused by the residual steam was 2.5% and it resulted in only a 1% difference between the theoretical and measured values. They concluded this was negligible.

Kuroki et al. also investigated the accumulation of impurities in the circulation gas. They found traces of NO_x , CO and HC which remained at almost undetectably low levels. However, they found that the concentration of CO_2 increased over time, produced from burning lubrication oil. CO_2 has a lower specific heat ratio than argon and a 15% concentration can reduce the cycle efficiency by 5% [8]. Although reducing the accumulation of CO_2 is a challenge, if it can be limited to 3%, the effect on the efficiency is less than 1%.

One potential advantage of APCs is their fuel flexibility. With the

addition of a CO_2 separator, they can burn small chain hydrocarbons such as methane. Chourou et al. [9] investigated the application of CO_2 membrane separation to an APC. The large difference in molecular weight between CO_2 and argon makes separation possible. They studied the effect of pressure ratio and CO_2 concentration in the working fluid on the energy consumption of the separation system. Their results show that maximum energy consumption occurs at low CO_2 concentrations but can be controlled by keeping the pressure ratio high. In the worst-case scenario, the efficiency penalty is 5% for a low concentration of CO_2 recirculating and less than 4% for a high concentration. It was concluded that the gain in efficiency of using a closed loop cycle justified the energy needed to separate the CO_2 .

There is also existing literature regarding the choice of noble gas used as the working fluid. Kusterer et al. [10] compared the performance of solar thermal Brayton cycles operated with helium and argon. They found that helium has the best thermal and transport properties owing to its low molecular weight. However, a low molecular weight increases the aerodynamic loading of the compressor blades, so more stages are needed to avoid the fluid boundary layer separating. Heavier noble gases (such as argon) have a lower heat capacity but a greater heat density meaning turbomachinery components need much fewer stages; this is ideal for lightweight applications and reducing cost. A similar investigation by El-Genk et al. [11] found that a binary mixture of He-Xe, with a molecular weight of 40 g/mol, exerted just 10% of the induced aerodynamic loading on the compressor and turbine blades that helium did. The penalty for the heavier working fluid was that 3.5 times as much compressor work was needed.

This work aims to determine the feasibility of using an APC for large scale power generation (>1 MW). A working Aspen Plus model has been produced based upon a modified closed-loop Brayton cycle that uses rotating turbomachinery to generate power. The model has been optimised for maximum efficiency and tested across a range of operating conditions with argon, helium and air as the working fluids and hydrogen and methane as the fuels.

2. Methodology

2.1. Cycle efficiency

The efficiency of a thermodynamic cycle is defined as the ratio of net work output to heat input. For a closed loop Brayton cycle, heat is added

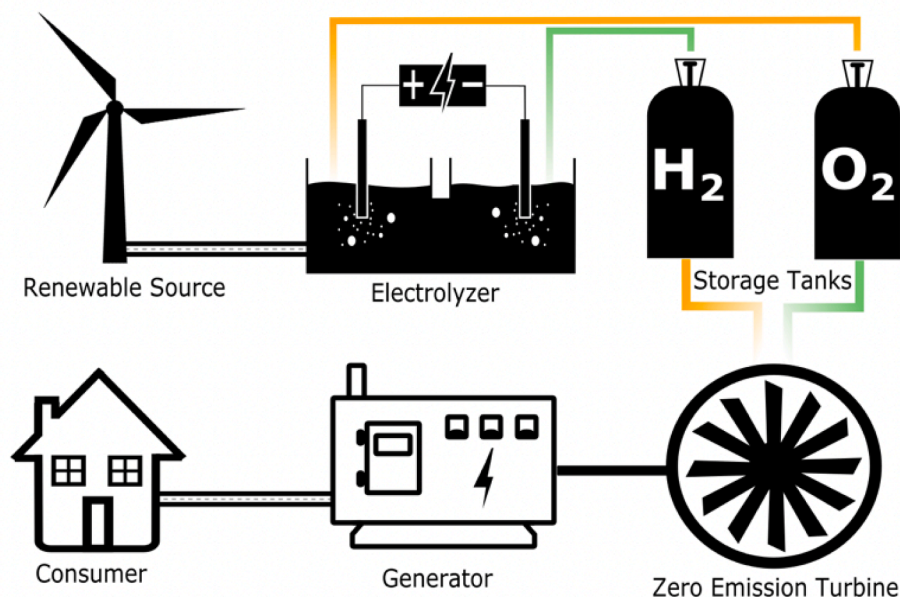


Fig. 1. Schematic of the 'hydrogen economy'.

from the combustion of the fuel. This is given by:

$$Q_{in} = HHV \cdot \dot{n} \quad (2)$$

The Higher Heating Value (HHV) for hydrogen is 286 kJ/mol [12]. Two efficiencies exist for the cycle: the electrical efficiency (η_e) which accounts for the electrical energy only and the electrical and thermal efficiency (η_{e+t}) which also accounts for the useful heat in coolant streams (Q_c). The estimated generator efficiency is 0.985 [13].

$$\eta_e = \frac{0.985 \cdot W_{net}}{Q_{in}} \quad (3)$$

$$\eta_{e+t} = \frac{0.985 \cdot W_{net} + Q_c}{Q_{in}} \quad (4)$$

2.2. Combustion

In the combustor, the fuel reacts with oxygen which releases energy to heat the outlet stream to the maximum cycle temperature. When hydrogen is the fuel, the following reaction occurs:



Looking at the molar ratio, it can be observed that the mole flow rate (MFR) of the hydrogen stream needs to be double that of the oxygen stream for complete combustion. If air is used to supply the oxygen, the air MFR needs to be calculated so complete combustion can still occur (Appendix 3.1.6).

2.3. The temperature ratio and pressure ratio

The relationship between the temperature ratio (T_{HP}/T_{LP}) and the pressure ratio (P_{HP}/P_{LP}) is summarised by Eq. (6), where HP and LP are high and low pressure locations respectively. The equation can be rearranged for T_{LP} :

$$\frac{T_{HP}}{T_{LP}} = PR^{\left(\frac{\gamma-1}{\gamma}\right)} \rightarrow T_{LP} = T_{HP} / PR^{\left(\frac{\gamma-1}{\gamma}\right)} \quad (6)$$

If the turbine inlet temperature (T_{HP}) is kept constant, the equation demonstrates that increasing the pressure ratio will reduce the turbine

outlet temperature (T_{LP}).

2.4. Determining the specific heat ratio

The number of Degrees of Freedom (DoF) of a gas determines the number of independent ways it can carry energy [14]. Monatomic gases can move in any direction in three-dimensional space and so have three independent translational DoF. Diatomic gases can move in space and rotate about two coordinate axes, giving them five DoF. Eq. (7) [14] links the number of DoF to the specific heat ratio:

$$\gamma = 1 + \frac{2}{DoF} \quad (7)$$

As demonstrated in Eq. (1), increasing the specific heat ratio of the working fluid increases the ideal efficiency. Argon is a monatomic gas and so has three DoF leading to $\gamma = 1 + 2/3 = 1.67$. Nitrogen and oxygen are both diatomic gases and so have specific heat ratios of 1.4. As the working fluid in an APC is a mixture of approximately 80% argon and 20% oxygen by volume, the specific heat ratio is 1.613. Table 1 details the standard operating conditions used in the analysis unless specified otherwise. The simulation is using the Wegstein method for convergence with the boundary conditions as tabulated in Table 2.

3. Standard Brayton cycle

A standard Brayton cycle consists of a compressor, combustor, and a turbine. To accommodate argon as the working fluid, the cycle must be closed loop to recirculate the argon and incorporates a condenser to remove the water, as shown in Fig. 3.

At position 1, oxygen is supplied to the cycle to make a gaseous mixture of argon and oxygen at the Reference Temperature and Pressure

Table 1
Standard operating conditions.

Condition	Value
Pressure Ratio	9
Fuel flow rate (kMol/s)	0.8
Working fluid flow rate (kMol/s)	4

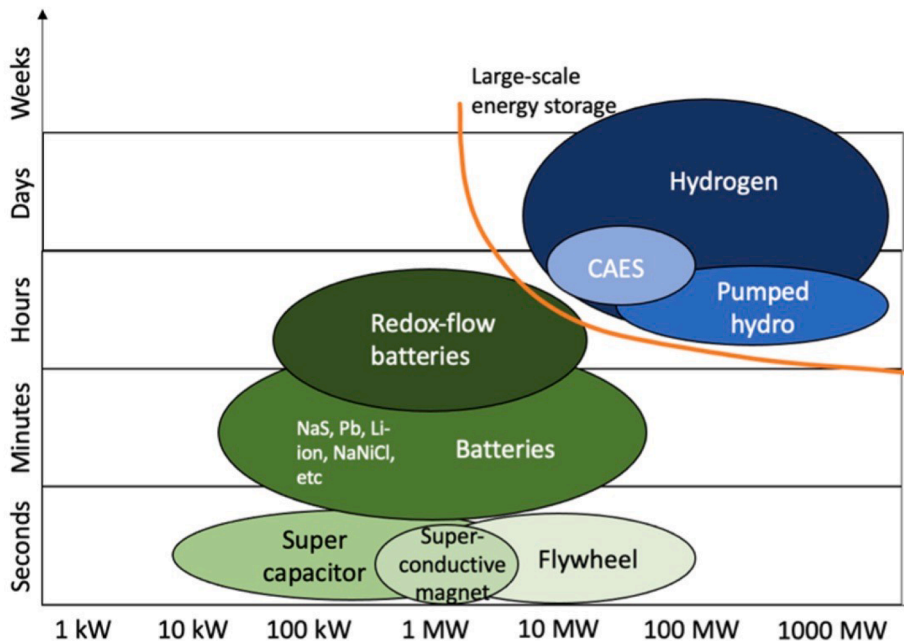
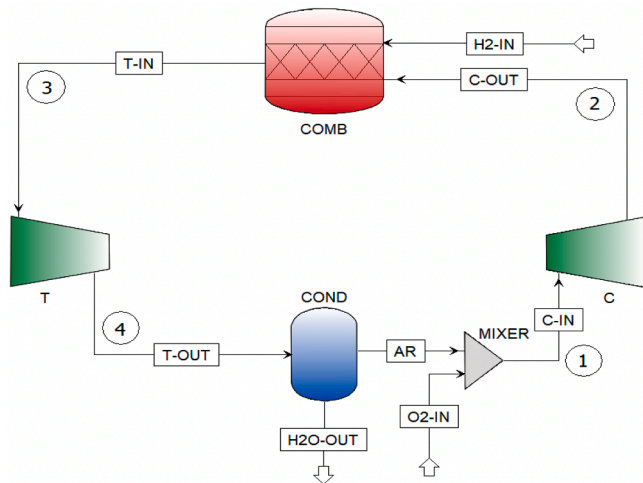


Fig. 2. Segmentation of electrical energy storage [6].

Table 2

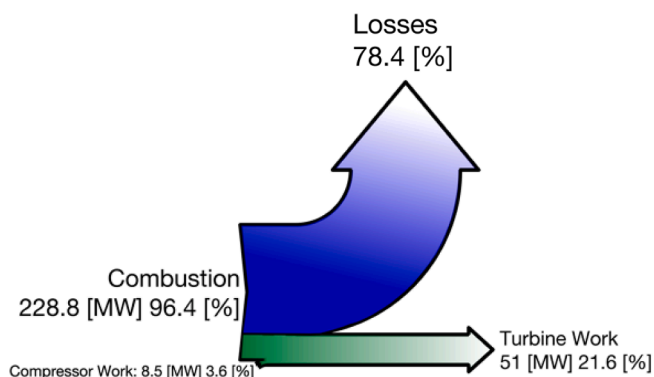
Boundary conditions.

Maximum flowsheet evaluations	100	
Wait (the number of direct substitution iterations before the first acceleration iteration)	1	
Consecutive direct substitution steps (number of consecutive acceleration iterations)	0	
Consecutive acceleration steps	1	
Wegstein acceleration parameters	Lower bound	–5
	Upper bound	0

**Fig. 3.** Standard Brayton cycle.

(RTP) nominally close to the ambient temperature. The pressure of the mixture is increased to the maximum in the compressor. In the combustor, high pressure hydrogen enters the cycle which reacts with the oxygen to produce heat and steam. This increases the temperature of the mixture before it expands through the turbine, converting heat into work that is used to drive the compressor. The excess work drives an external electricity generator. Finally, before recirculation, water is separated from the argon in the condenser.

This cycle has been modelled, to provide a benchmark from which to build upon. Under standard conditions (Table 1), the maximum efficiency achieved is 19%. This is because the exhaust stream from the turbine still carries a lot of heat. When it is directly connected to the condenser, all of that heat is lost as the steam cools and liquifies. The Sankey diagram in Fig. 4 shows the power flow through the system.

**Fig. 4.** Power flow through the standard Brayton cycle.

3.1. Improvement methods

The key to unlocking the efficiency of the cycle is to extract as much power as possible out of the hot exhaust stream before it can enter the condenser. Modifying the standard Brayton cycle involves adding extra components resulting in a compromise between the possible efficiency gain and extra system cost. Due to material limitations, in this work and for simplicity, it has been considered that it is not viable to have a turbine inlet temperature to exceeding 1873 K [13], so the combustor outlet stream must not exceed this figure. In order to achieve this without sacrificing efficiency, one possible modification is the addition of a water spray chamber. Wastewater from the condenser is collected and sprayed into a chamber where it mixes with the combustor outlet stream. The water evaporates, absorbing energy and reducing the temperature of the stream to an acceptable 1873 K. The mass flow rate of the stream through the turbine is also greater which increases its power output.

To take full advantage of the heat in the exhaust, a Heat Recovery Steam Generator (HRSG) can be added. The exhaust stream passes through a heat exchanger which heats pressurised water to steam for use in an external Rankine cycle. The steam then expands through a turbine to generate extra work. Rankine cycles have a reported efficiency of approximately 20% [15], which can be used to increase the efficiency of the whole system to 34% when operating under standard conditions (Table 1). It should be noted that external cycles would represent a costly modification and so may only be feasible for larger scale power generation applications where the up-front cost is more justifiable.

The most promising Brayton cycle modification is the incorporation of a regenerator. This uses the hot exhaust gases to preheat the combustor inlet stream so that less heat needs to be added from combustion to achieve the same outlet temperature. For the regenerator to work optimally, a large temperature difference is needed between the turbine and compressor exhausts. This requires an extra turbine and compressor with heat exchangers located between them. The inlet to the second compressor is intercooled back to ambient, this minimises the compressor exhaust stream temperature and the power consumption. The outlet of the first turbine is then reheated to 1873 K to maximise the exhaust stream temperature and the power output. Fig. 5 shows the modified cycle configuration.

Fig. 6a depicts the Temperature-Entropy profile for a standard Brayton cycle. The effect of the modifications can be observed by studying the modified Temperature-Entropy diagram as illustrated in Fig. 6b. The turbine outlet temperature (8) is maximised through reheat and the compressor outlet temperature (4) is minimised through intercooling. This increases the gap between (4) and (*); the temperature rises due to regeneration. Hence, to achieve the same maximum cycle temperature, combustion only needs to increase the temperature from (*) to (5), a solution which uses less fuel.

Preliminary calculations to assess the feasibility of the regeneration modifications shows that under standard conditions, an efficiency of 55% is possible.

4. Hydrogen-Argon model development

Appendix 1 shows the full layout hydrogen-argon model; however, it can be summarised as starting from pure argon in the 'AR' stream, oxygen is added at RTP before the first stage of compression. Compression naturally raises the outlet temperature and so the intercooler cools it back down to ambient. After the second stage of compression, the stream enters the regenerator where it is preheated to the temperature of the exhaust gases. Extra heat is then added from the combustion of hydrogen and oxygen to reach the maximum cycle temperature. The stream then passes through a splitter and into a spray chamber where enough water is added to cool the temperature down to 1873 K. After expansion in the first turbine, the stream is reheated to as close to 1873 K as possible before the second expansion. The exhaust stream passes back

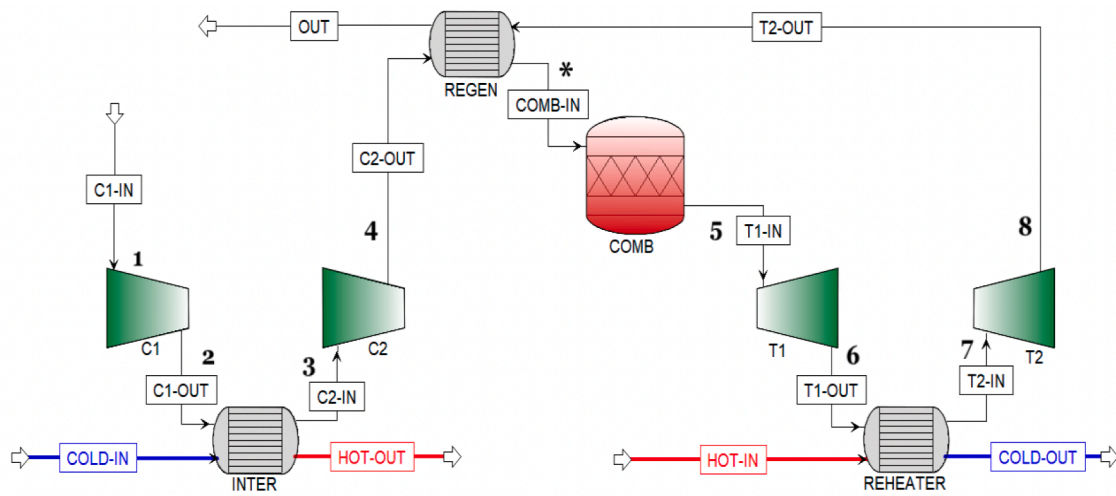


Fig. 5. Modified Brayton cycle configuration.

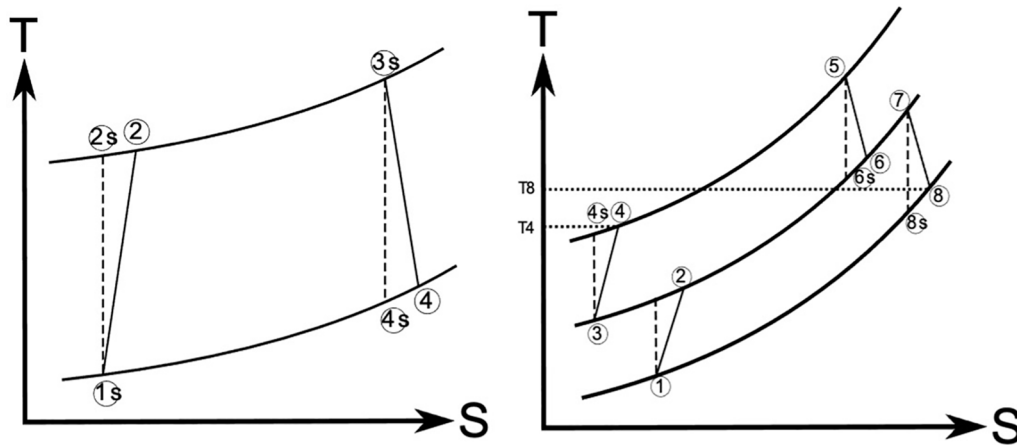


Fig. 6. Temperature-Entropy diagram of (a) the standard Brayton cycle and (b) the modified Brayton cycle.

through the regenerator and a heat extractor which takes more heat out of it before it enters the condenser. Here, the water is extracted leaving high purity argon for recirculation. The extracted water enters a cooling circuit, starting with the intercooler and then a splitter. This splits the stream, so the correct amount is sent to the spray chamber with the remainder sent to the final heat exchanger to extract heat from the exhaust. The hot water outlet can be utilised externally.

The following design modifications also improved performance:

- Recycling the water from the condenser as the coolant reduces the number of inputs and outputs, eliminating the need for external coolant sources.
- Using a water spray chamber rather than a heat exchanger to cool the turbine inlet stream increases the mass flow rate and therefore the power output of the turbines.
- A 'HOT OUT' stream after the combustor enables the cycle to be flexible in the amount of heat and work it produces. For this analysis the flow rate of the 'HOT OUT' stream is zero, but the cycle could produce 100% heat if required.
- When the steam cools and liquifies in the condenser, a large amount of heat is released. To prevent this from being wasted, a 'HEAT' stream carries it to a secondary circuit that supplies the reheater. Although heat streams only exist in ideal scenarios, in practice, cooling pipes around the condenser can be used to transfer the heat to the reheater.

- The pressure ratios across the pair of compressors and turbines are equal. This means that they perform identically under standard conditions.

4.1. Performance analysis

Argon 'mole flow rate (MFR)' was initially 2 kMol/s and subsequently increased up to 8 kMol/s through steps of 2 kMol/s increments. At each stepping, power output and efficiency data were recorded for different pressure ratios. In Fig. 7, the solid lines show the electrical efficiency only and the dashed lines show the electrical and thermal efficiency by accounting for the heat in the 'H₂O-OUT' stream. The dotted lines show the net power output. The following observations can be made:

- A. The efficiency increases as the Ar MFR increases.

At high argon MFRs, a higher fraction of the available heat from the condenser can be used for reheating so less is wasted.

- B. Between pressure ratio 4 and 10 the efficiency increases linearly for all Ar MFRs. It then plateaus for the Ar MFR less than 8 kMol/s cases.

The efficiency increases in accordance with the ideal Brayton cycle

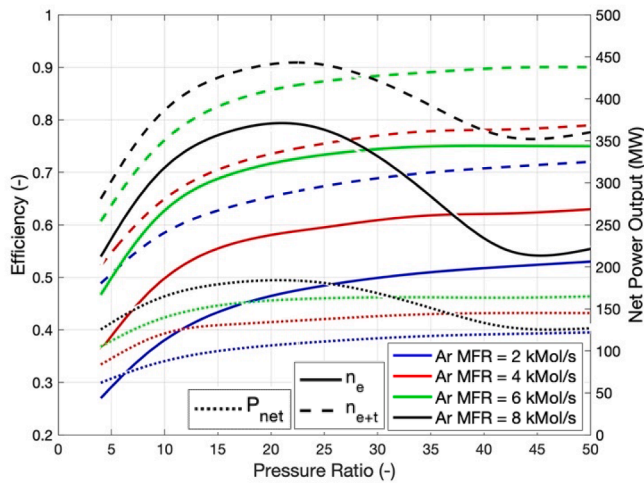


Fig. 7. –Performance of the hydrogen-argon cycle.

efficiency (Eq. (1)). The plateaus are caused by the increase in compressor work that is needed to produce the higher pressure-ratios.

- C. When the Ar MFR = 8 kMol/s, the efficiency and net power output peak at pressure ratio 24 and then decrease.

At high argon MFRs and high pressure-ratios, the compressors consume a lot of power and so the exhaust streams are hot. This means that a greater heat duty is required from the intercooler to restore the temperature to ambient; at pressure ratios exceeding 24 the intercooler cannot achieve this (Appendix 1.3). When this happens the inlet to the second compressor is above ambient temperature and its density decreases, in accordance with Eq. (8).

$$\rho = \frac{P}{RT} \quad (8)$$

A less dense gas requires more work to compress, resulting in a hotter inlet stream at the ‘cool’ side of the regenerator. On the ‘hot’ side of the regenerator, the turbine exhaust temperature decreases as the pressure ratio increases (Eq. (6)). Both effects mean the temperature difference across the regenerator is lower, less heat is transferred back into the cycle and more has to be rejected in the condenser. There is no change to the heat added by the fuel, so a cooler combustor inlet means the outlet is also cooler. This reduces the cycle temperature ratio and so the efficiency decreases.

- D. After reaching a minimum at pressure ratio 42, the efficiency and net power output of the Ar MFR = 8 kMol/s case increases again.

At a pressure ratio of 42, the temperature difference across the regenerator is approaching zero so it is redundant, and the efficiency reaches a minimum of 54% (Appendix 1.3). If the pressure ratio is increased further, the regenerator and intercooler remain redundant and the cycle behaves like the standard Brayton cycle. That means the efficiency is governed only by Eq. (1), leading to the slight increase in efficiency observed.

When the argon MFR is 8 kMol/s, the optimal operating point is at a pressure ratio of 24. Either side of this, the intercooler and regenerator are not working optimally. Although efficiency starts to increase again at pressure ratios >42, this is less practical to achieve.

Fig. 8 depicts the net power output of the cycle when Mole Flow Rate of the fuel is varied. To satisfy the stoichiometric ratio in Eq. (5), the oxygen MFR is always half the hydrogen MFR.

The following observations can be made:

- A. The net power output of the H₂ MFR = 0.2 kMol/s case decreases to a minimum and then stabilises as the pressure ratio increases.

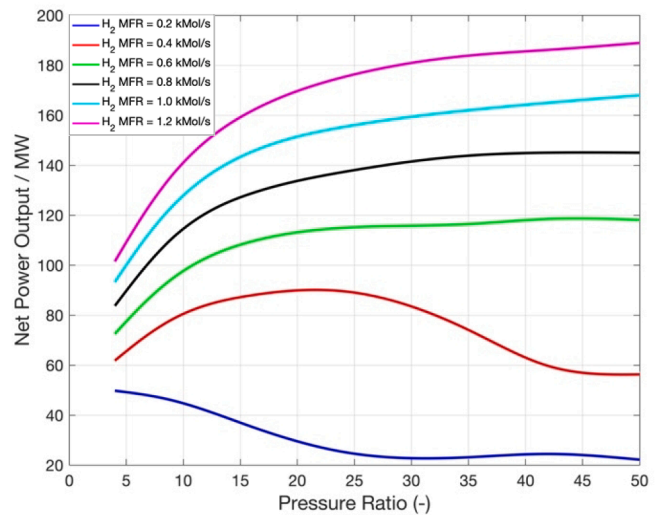


Fig. 8. Variation of the net power output with the change in fuel flow rate.

The heat required to increase the combustion temperature at a fixed amount increases with the pressure ratio. Therefore, at low pressure ratios, low fuel flow rates can produce high cycle temperatures and the regenerator works effectively. As the pressure ratio increases, the heat requirement increases until the maximum cycle temperature drops below 1873 K at a pressure ratio of approximately 6. From this point, no cooling water is needed in the spray chamber and the power output from the first turbine reduces which means the net power output reduces.

As the pressure ratio approaches 30, the compressors require more power, which requires a greater heat duty from the intercooler to restore the intermediate stream temperature back to ambient. However, a low fuel flow rate means very little water is produced in the combustion chamber for the intercooler to use and so it fails because it cannot meet its target of cooling the stream to ambient. Hence, the inlet and outlet temperatures of the second compressor start to increase.

As the pressure ratio is increased further still, the rising compressor outlet temperature exceeds the turbine exhaust temperature causing the regenerator to fail. However, rising temperatures actually have a positive effect, because when the combustor outlet temperature exceeds 1873 K, water is needed in the spray chamber again. Introducing more water into the cycle provides more coolant for the intercooler so the second compressor exhaust temperature begins to decrease, and it consumes less power. Hence, the net power output stabilises.

- B. The net power output of the H₂ MFR = 0.4 kMol/s case increases up to a maximum at PR = 20, then decreases and stabilises as the pressure ratio increases further.

A greater fuel flow rate increases the maximum cycle temperature and the water needed in the spray chamber. This means the mass flow through the turbines is higher and they produce more power, hence increasing the net power output. When compared to the H₂ MFR = 0.2 kMol/s case, the cycle is able to reach a higher pressure-ratio (PR20) before the combustor outlet temperature drops below 1873 K. At pressure ratios beyond this, the net power output decreases and then stabilises for the same reasons explained previously.

- C. For higher fuel flow rates (H₂ MFR > 0.4 kMol/s), the net power output plateaus at higher pressure ratios.

Higher fuel flow rates mean that more cooling water is available to prevent the intercooler from failing in the tested range of pressure ratios. Instead, it is the increase in compressor work that causes the plateau. It can be expected that at pressure ratios high enough, the intercooler will fail and the same decrease and stabilisation in net power output that was observed for lower fuel flow rates will occur.

4.2. Model limitations

- At high working fluid flow rates and low fuel flow rates, the combustor outlet stream temperature can drop below 1873 K. This reduces the maximum possible power output from the first turbine and hence reduces the efficiency.
- At higher working fluid flow rates a lot of heat is needed to reheat the input to the second turbine back up to 1873 K. When this exceeds the heat available from the condenser, the stream temperature drops below 1873 K, reducing the power output from the second turbine and the cycle efficiency.
- The cycle extracts water produced from combustion in the condenser as coolant for the intercooler, spray chamber and heat extractor. When the fuel flow rates are very low, there is not enough water formed to prevent the intercooler from failing at high pressure ratios. The result is that the inlet to the second compressor is hotter and it consumes more power, reducing the net power output and efficiency.
- At high pressure ratios, the compressor work is high and so is the outlet temperature from the second compressor. If the fuel flow rates are also low, the turbine exhaust temperature can drop below the compressor exhaust temperature. In this scenario heat is transferred backwards across the regenerator, cooling the combustor inlet, and heating the condenser inlet.

5. Case study 1: Hydrogen – Helium cycle

To combat some of the aforementioned limitations and further understand the performance of the cycle, different fuels and working fluids have also been explored. The first case study investigates a hydrogen–helium cycle to explore the effect of the choice of noble gas on performance (Appendix 2.1).

A major difference is that less compressor work is required in the hydrogen–helium cycle. Under standard conditions (Appendix 2.2), the pre-compressor molar composition of the hydrogen–helium cycle is 89% helium and 9% oxygen with a mass composition of 52% helium and 42% oxygen. The difference between the mass and molar composition is because helium molecules are much lighter than oxygen molecules. The heat capacities (c_p) of helium and oxygen are $5.2\text{J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ and $0.92\text{J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ respectively. Therefore, the presence of oxygen in the mixture decreases the heat capacity to $3.2\text{J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$. For comparison, the hydrogen–argon cycle pre-compressor mass composition is 91% argon and 7% oxygen. The heat capacity (c_p) of argon is $0.52\text{J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$, so the presence of oxygen increases the heat capacity of the mixture to $0.56\text{J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$.

The comparative molecular weights of argon and helium mean the mass flow rate (\dot{m}) of the helium stream is lower, despite the mole flow rates being the same. This difference, coupled with the reduced heat capacity for the helium–oxygen mixture, means that the compressors require less power (\dot{W}_c). Eq. (9) links these variables.

$$\dot{W}_c = \dot{m}c_p(T_2 - T_1) \quad (9)$$

5.1. Performance analysis

Performance of the hydrogen–helium cycle is shown in Fig. 9. The following observations can be made between the hydrogen–helium and hydrogen–argon models:

- The efficiency does not experience the same rate of reduction at high pressure ratios and high helium MFRs.**

As stated previously, the work required to compress the same MFR of helium is less than for argon. Therefore, the first compressor outlet stream is cooler, and the heat duty required from the intercooler to restore it to ambient is less. This means higher pressure ratios can be

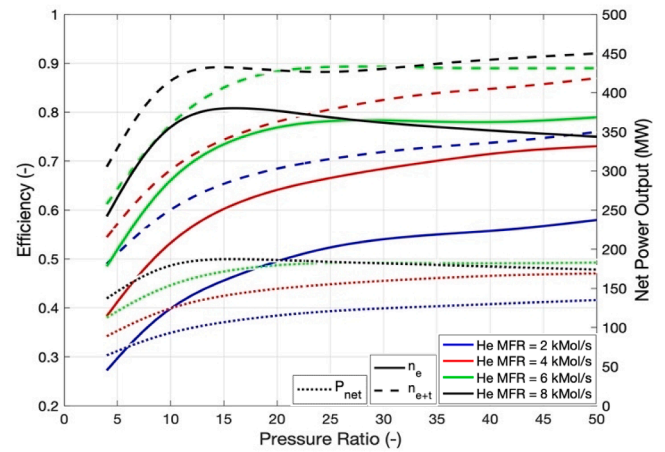


Fig. 9. Performance of the hydrogen–helium cycle.

achieved in the hydrogen–helium cycle before the intercooler fails.

B. The efficiency peaks and plateaus at lower PRs.

In the hydrogen–argon cycle, there is always enough heat available from the condenser to reheat the inlet of the second turbine back up to 1873 K because the intercooler fails before the reheater does. However, in the hydrogen–helium cycle, a critical pressure ratio is reached, beyond which the second turbine inlet temperature is no longer limited by the 1873 K material condition, but by the heat available from the condenser (Appendix 2.3). Higher pressure streams require more reheating; hence the second turbine inlet temperature decreases as the pressure ratio increases. This effect is balanced by the natural efficiency increase at higher pressure ratios, causing the plateau. It can be expected that the intercooler will still fail but at a very high pressure-ratio (>50) and will result in a similar dip in efficiency as is observed in the hydrogen–argon case.

C. When the helium MFR = 8 kMol/s, the electrical and thermal efficiency streams diverge at high pressure ratios.

In the hydrogen–argon cycle it was apparent that once the intercooler fails, the combustor outlet temperatures start to increase. This requires more water in the spray chamber to cool the turbine inlet stream, so less is available for the thermal stream. This is different to the hydrogen–helium cycle which follows the expected trend of the combustor outlet temperature decreasing as the pressure ratio increases. Therefore, less water is needed in the spray chamber and more is available for the thermal stream, accounting for the divergence.

D. The net power outputs are generally higher than was observed for the hydrogen–argon cycle.

Helium and argon are both monatomic gases and therefore have the same specific heat ratio. Recalling Eq. (6), this means that at the same pressure ratio they will produce the same temperature ratio across the turbines. When the working fluid MFR is also the same, both cycles produce the same turbine power, this can be observed by comparing the dashed lines in the two power graphs. As explained previously, the compressor work is lower across all pressure ratios for the hydrogen–helium cycle which accounts for the net power output being greater.

6. Case study 2: Hydrogen – Air cycle

It is important to investigate the cycles performance using air as the

working fluid given its ease of use and infinite, free supply. The cycle will not require a separate oxygen supply, so the model has been adapted to be open loop (Appendix 3.1). This enables fresh air to continuously replace the oxygen as it is consumed in the combustor. The working fluid in open loop cycles is fixed at atmospheric conditions and so the cycle loses some of its flexibility. The air is modelled as 23% oxygen and 77% nitrogen by mass (Appendix 3.1.6). Although there will still be zero production of carbon dioxide, having nitrogen present at the high temperatures in the combustor will produce some NO_x gases so the cycle is not strictly zero emission.

6.1. Performance analysis

Performance of the hydrogen-air cycle is depicted in Fig. 10. As nitrogen makes up the majority of air, it is reasonable to assume it to be the working fluid in the hydrogen-air cycle.

The following observations can be made between the hydrogen-air model and previous models:

A. The compressor power is lower than was observed for the hydrogen-argon cycle (Appendices 1.2 and 3.2).

Similarly, to the hydrogen-helium cycle, the compressors in the air cycle consume less power than the compressors in the hydrogen-argon cycle, but the reasoning is different because nitrogen and argon are more similarly sized molecules. Nitrogen is a diatomic gas so has a specific heat ratio of 1.4, which is lower than that of argon. Recalling Eq. (6), the temperature ratio is dependent upon the specific heat ratio. Hence, for a constant pressure ratio and inlet temperature (T_{LP}), the compressor outlet temperature (T_{HP}) is lower for the hydrogen-air cycle. A lower temperature difference means the compressors require less power as is demonstrated in Eq. (9). The same reasoning can be used to explain why the turbine power output is lower for this cycle.

B. The efficiency is more stable at high pressure ratios and air MFRs.

The intercooler in the air cycle does not fail at high pressure ratios and a working fluid MFR of 8 kMol/s because of the reduction in compressor power. This is the same reason as was discussed for the hydrogen-helium cycle. Therefore, the second turbine inlet temperature is determined by the heat available from the condenser rather than the 1873 K material specification (Appendix 3.3). This becomes the limiting factor and balances the efficiency increase caused by an increase in pressure ratio. Even though the efficiency plateaus, the turbine power

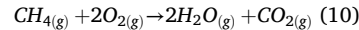
output continues increasing, just at a slower rate because the second turbine is producing less power than the first.

C. The efficiency is lower across all pressure ratios.

The lower efficiencies found in this case study stem from the extra DoF of nitrogen and its lower specific heat ratio (Section 3.4). This results in a greater proportion of the heat supplied to the gas being converted into internal energy and therefore not able to do work [14].

7. Case study 3: Methane - Argon cycle

To bridge the gap between current technology and the future hydrogen economy, it is desirable for the model to be powered cleanly from fossil fuels. Methane is a short chain hydrocarbon with a HHV of 889 kJ/mol [12]. Burning methane produces carbon dioxide which needs to be removed from the cycle before recirculation. The cycle has been modified to include a carbon dioxide separator after the condenser (Appendix 4.1). The carbon dioxide that is removed is very pure and can be captured for underground storage, thereby meeting the specification of zero emissions. Methane and oxygen react in the following way:



7.1. Performance analysis

Performance of the hydrogen-air cycle is portrayed in Fig. 11. The following observations can be made between the methane-argon model and previous models:

A. Over all pressure ratios, the efficiency is lower, but the net power output is higher.

The much larger HHV for methane means that for every mole of fuel burnt, a larger amount of heat is added to the cycle. This raises the cycle temperatures and so more cooling water is needed in the spray chamber which increases the mass flow through the turbines and hence their power outputs. Despite this, the proportion of heat input to work output is lower than in the hydrogen models and therefore the efficiencies are lower.

B. The extent of reaction for the methane-argon cycle is 0.8 compared to 0.4 for the hydrogen cycles.

From the stoichiometric ratio in Eq. (10), each methane molecule needs to find two oxygen molecules to produce water. Whereas in the

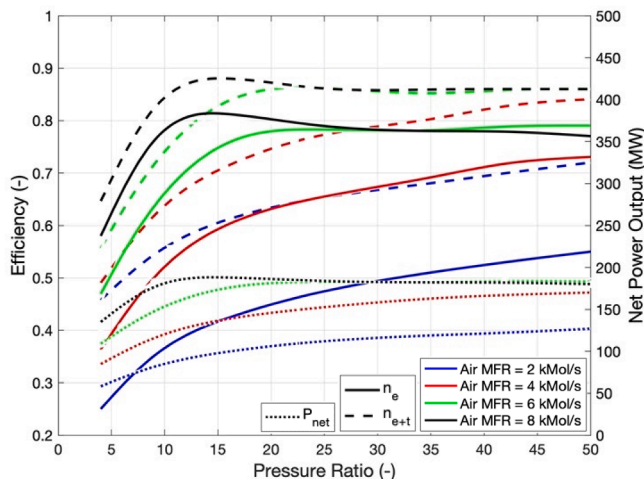


Fig. 10. Performance of the hydrogen-air cycle.

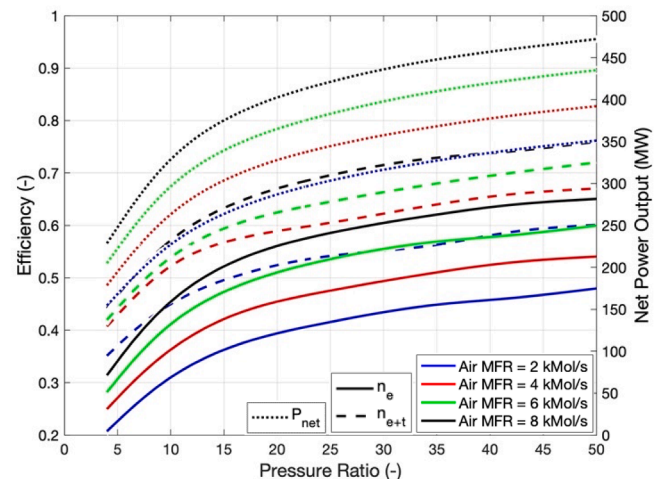


Fig. 11. Performance of the methane-argon cycle.

hydrogen cycles, two hydrogens need to find one oxygen to produce water. The MFRs of both fuels are the same, meaning that for complete combustion, 1.6 kMol/s of oxygen is needed for the methane cycle and 0.4 kMol/s of oxygen for the hydrogen cycles. Therefore, it is relatively easier for one methane to find two oxygen molecules than it is for two hydrogens molecules to find one oxygen molecules. The result is that water is formed twice as quickly in the methane-argon cycle.

C. There is no decline in efficiencies at high pressure ratios and high argon MFRs.

Having twice the MFR of water in the methane cycle has two consequences. Firstly, there is sufficient cooling water to prevent the intercooler from failing at high pressure ratios. Secondly, there is sufficient heat produced in the condenser to reheat the second turbine inlet stream back up to 1873 K, even at elevated conditions, therefore preventing the reheater from failing. The absence of these two failure modes that were present in the hydrogen cycles explains why the efficiencies begin to plateau at a much greater pressure ratio (Appendix 4.3). The only factor preventing the efficiency from increasing indefinitely is the increase in compressor work.

D. Less compressor power is required than for the hydrogen-argon cycle.

When operating under standard conditions, the pre-compressor mass composition in the methane-argon cycle is 75% argon and 24% oxygen. For the hydrogen-argon cycle, it is 91% argon and 7% oxygen. Oxygen is a diatomic gas and its presence in argon reduces the specific heat ratio of the mixture. This is more significant in the methane-argon stream and it reduces the specific heat ratio from 1.67 to 1.55. The consequence of this can be observed using Eq. (6) if T_{HP} and T_{LP} are taken to be the outlet and inlet of a compressor respectively. For a constant inlet temperature, a lower specific heat ratio leads to a lower outlet temperature, this can be observed in Appendix 4.2. The result is a lower temperature difference across the compressors, and they require less power (Eq. (9)).

8. Power flow analysis

A deeper understanding of how the cycles are performing can be gained by looking at the Sankey diagrams which visually show the power flow through the system. Fig. 12 and Table 3 compares the performance of each cycle at maximum efficiency operation with a working fluid MFR of 8 kMol/s.

The 'Losses' output stream represents heat that is available from the condenser but not needed in the reheater. As presented in Section 7.1.B, the methane-argon cycle produces water at twice the rate of the hydrogen fuelled cycles and hence more heat is available in the condenser. The reheater does not need all of this heat and so a larger proportion of it is lost.

The 'Heat' output stream refers to the heat removed from the cycle in the 'H₂O-OUT' stream. This is high grade heat that can be used in industrial processes or diluted for domestic heating [16]. In large scale systems, it may be economically feasible to utilise the heat in a HRSG and generate extra power.

Aspen Plus is an idealised software which neglects some sources of loss, such as friction losses, mechanical losses and unwanted heat transfer. In reality, these sources will feature as extra independent outputs on the Sankey diagram and reduce the cycle efficiency. The magnitude of these losses will increase as the power output of the cycle increases.

9. Economic analysis

Under standard conditions the cycles can be compared by investigating their Operating Expenditure (OPEX) and Capital Expenditure

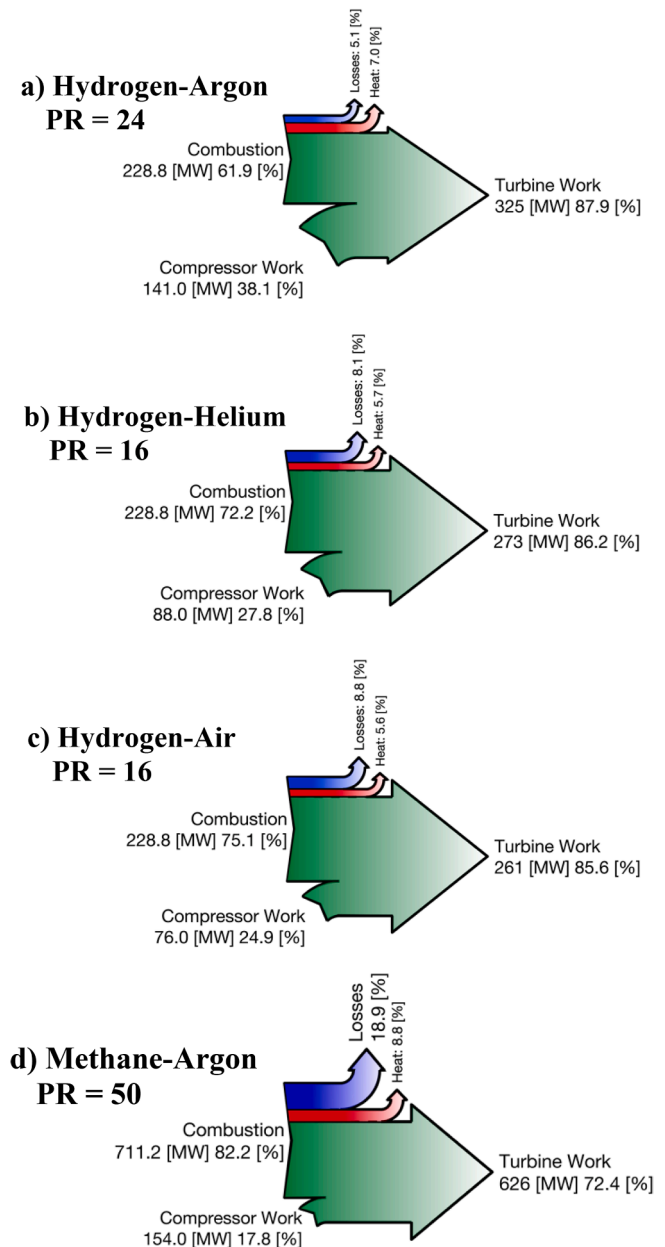


Fig. 12. Power flows at maximum efficiency operation.

(CAPEX). The OPEX (Table 4) consists of the materials that are consumed in the cycle. The prices shown are per kWh of heat and electricity generated by the system. As a reference, the average cost of non-domestic electricity in the UK in 2020 was £0.1/kWh [17].

Ideally, the working fluid is not consumed and is therefore included in the CAPEX. However, in a worst case scenario, 5% of the total flow rate might be expected to leak from labyrinth seals separating the components [22], this fraction has been accounted for in the OPEX. The working fluid represents a significant proportion of the cost because of the large MFRs required.

Table 4 shows that only the hydrogen-air cycle can currently compete with the cost of non-domestic electricity in the UK. This is because of the high costs of bottled oxygen, argon, and helium. However, oxygen is a by-product of the electrolysis of water. Therefore, it is expected that as renewable integration increases and a greater proportion of excess energy is utilised in water electrolysis, the cost of oxygen will decrease. The cost of the working fluids is likely to be more constant but can be minimised by capturing and recycling leakage flows.

Table 3

Inputs and outputs for all the cycles at maximum efficiency operation.

	Pressure Ratio	Working Fluid MFR (kMol/s)	Inputs		Outputs		
			Combustion (MW)	Compressor Work (MW)	Losses (MW)	Heat (MW)	Turbine Work (MW)
Hydrogen-Argon	24	8	228.8	141	5.1	7	325
Hydrogen-Helium	16	8	228.8	88	8.1	5.7	273
Hydrogen-Air	16	8	228.8	76	8.8	5.6	261
Methane-Argon	50	8	711.2	154	18.9	8.8	626

Table 4

OPEX for each cycle.

Parameter	Quantity (kMol/s)	Rate (£/kg)	Cost (£/kWh)
Hydrogen-Argon			
Hydrogen	0.8	2.18 [4]	0.08
Oxygen	0.4	1.45 [18]	0.45
Argon	0.2	5.85 [19]	1.13
Total	–	–	1.66
Hydrogen-Helium			
Hydrogen	0.8	2.18	0.08
Oxygen	0.4	1.45	0.43
Helium	0.2	212.01 [20]	3.91
Total	–	–	4.42
Hydrogen-Air			
Hydrogen	0.8	2.18	0.09
Total	–	–	0.09
Methane-Argon			
Methane	0.8	0.98 [21]	0.13
Oxygen	1.6	1.45	1.56
Argon	0.2	5.85	1.69
Total	–	–	3.38

10. Conclusion

In this study, a novel closed loop modified Brayton cycle has been researched and developed. Simulations have been carried out to understand how the model performs across a range of pressure ratios, working fluid flow rates and fuel flow rates. A hydrogen-argon model was first developed and tested. To determine the flexibility of the model, three case studies have been investigated: a hydrogen-helium, hydrogen-air, and hydrogen-methane model. Each case study has its own unique advantages. The hydrogen-helium cycle is more efficient over all pressure ratios, but the gas is 36 times more expensive than argon per kg. The hydrogen-air cycle requires no additional working fluid and can be open loop, making it the cheapest to build and operate. However, flexibility is sacrificed, it is less efficient, and the formation of NO_x gases fail to meet the zero-emission specification. The methane-argon cycle is also less efficient but produces a significantly higher work output, making it favourable where efficiency isn't the highest priority.

11. Future scope of work

The ZECCY relies on hydrogen produced from renewable sources through electrolysis. Research needs to be carried out to determine the feasibility and time scale of PEM electrolysis to produce hydrogen on the scale that is needed. An economic analysis of the whole electrolysis – storage – ZECCY system needs to be carried out to determine capital expenditure, payback times and expected revenues. It would also be useful to look at some specific applications where a ZECCY could be used and how feasible it would be. For example, to power large ships, to replace a certain sized power station, to power a certain sized community. As the hydrogen produced from electrolysis can be fairly easily transported, the ZECCY doesn't need to be close to the electrolyser which adds a lot of potential/flexibility.

CRedit authorship contribution statement

Matthew Hodgson: Methodology, Software, Investigation, Writing - original draft. **Sumit Roy:** Conceptualization, Writing - review & editing. **Anthony Paul Roskilly:** Funding acquisition, Writing - review & editing. **Andrew Smallbone:** Supervision, Resources, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.enconman.2021.114510>.

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